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Applying Metrological Techniques to Satellite Fundamental Climate Data Records

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Abstract. Quantifying long-term environmental variability, including climatic trends, requires decadal-scale time series of observations. The reliability of such trend analysis depends on the long-term stability of the data record, and understanding the sources of uncertainty in historic, current and future sensors. We give a brief overview on how metrological techniques can be applied to historical satellite data sets. In particular we discuss the implications of error correlation at different spatial and temporal scales and the forms of such correlation and consider how uncertainty is propagated with partial correlation. We give a form of the Law of Propagation of Uncertainties that considers the propagation of uncertainties associated with common errors to give the covariance associated with Earth observations in different spectral channels.

1. Introduction

Satellite-derived Earth Observation (EO) data provide a legacy of information about environmental and climate changes that is of immense value to society. Obtaining information about long-term trends requires the comparison of satellite-derived observations taken decades apart, using different sensors and often the combination of data from sensors measuring in, e.g. different regions of the electromagnetic spectrum. To ensure that such comparisons are meaningful, it is essential to quantify the stability of satellite sensors and to determine the radiometric differences between different sensors and their associated uncertainties.

Some satellite series have been available for almost 40 years, the first versions of which were launched in the late 1970s. Each satellite had a limited lifetime, and therefore a series of such satellites were launched, often with identical sensors on board, or with newer instrument generations that were an evolution of earlier designs. The operational calibrations of such sensor series were not intended for climate applications – for example, they are not stable over time. However, they made measurements over a time of significant climate change and the records from their observations, though currently not fit for purpose, are of great interest for our understanding of the Earth's environment.

Metrological principles of traceability, uncertainty analysis and comparison can be used to quantify long-term stability of Fundamental Climate Data Records (FCDRs); i.e. multi-decadal observations of fundamental quantities (such as top-of-atmosphere Earth radiance) from multi-satellite series. However, techniques established for laboratory calibrations cannot translate directly into Earth observation applications. The process of launch and natural degradation in space, along with the lack of SI-traceable references in orbit means that traceability is lost after launch. With historical sensors, particularly those

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launched in the 1980s – 90s, there is often also insufficient accurate information available from the pre-flight calibrations to perform a complete uncertainty analysis. Furthermore, in orbit, repeat measurements are generally not available since the turbulent and chaotic atmosphere modifies the top of atmosphere radiance observed from space.

In this paper we discuss approaches defined within the FIDUCEO project [1] for applying metrological techniques to FCDRs in the visible, thermal infrared and microwave spectral regions, We also introduce some concepts for the next step: the application of these FCDRs to generate Climate Data Records (CDRs) of geophysical products, with as rigorous uncertainty analysis. This paper is a conference proceedings paper and the ideas will be further elaborated in a paper in preparation [2].

Considered also is how we can provide a better calibration of the instrument, based on what we know now, and how we can establish more rigorous uncertainty analysis for the observations from such sensors in order to develop FCDRs. The recalibration process, harmonisation, involves the determination of new calibration coefficients for the instrument, either to improve the information available from pre-flight calibration, or to estimate quantities that were not determined pre-flight. Harmonisation is achieved using match ups: where a particular satellite sensor observed the same Earth scene as another sensor at the same time and in similar spectral bands/viewing angles.

The development of an FCDR then involves three main steps: (1) the establishment of a measurement equation, which is used to convert the observed counts into the FCDR quantity (e.g. radiance); (2) the analysis of the uncertainty associated with each quantity in the measurement equation, and the error correlation structure for the effects that influence each quantity; and (3) the harmonisation of the series. In the following sections we discuss these steps.

2. The measurement equation

We start our analysis of an FCDR with the measurement equation for the sensor, which converts the measured detector counts (the Level 0 product) into radiance or reflectance (the Level 1 product). It may be appropriate to use a different measurement equation for historical reanalysis than that which was used for the production of operational data, allowing for additional effects to be taken into account. For example for the AVHRR (Advanced Very High Resolution Radiometer) instrument, onboard the NOAA (National Oceanic and Atmospheric Administration, USA) satellite series since 1978, the (simplified) measurement equation [3] takes the form

$$L_{\mathrm{E}} = a_0 + \frac{(\varepsilon + a_1) L_{\mathrm{ICT}} - a_2 \tilde{C}_{\mathrm{ICT}}^2}{\tilde{C}_{\mathrm{ICT}}} C_{\mathrm{E}} + a_2 C_{\mathrm{E}}^2 + 0 \qquad (1)$$

where L_{E} is the Earth radiance observed by a particular instrument channel and for a particular image pixel; C_{E} is the measured Earth count for that pixel; L_{ICT} is the radiance of the internal calibration target (ICT) in that channel; $\tilde{C}_{\mathrm{ICT}}$ is the measured (averaged) signal from observing that ICT; ε is the emissivity; the different a_i are harmonised calibration parameters and 0 represents effects relating to the assumptions implicit in the form of the measurement equation. In general, the calibration parameters will be estimated through a combination of pre-flight calibration (here, emissivity ε), in-flight calibration (in this case the gain – the term in front of the linear counts term – which is determined from the ICT radiance and counts) and, for historical sensor series, through harmonisation (here, the a_i). Harmonisation is the process of determining improved calibration parameters for a series of satellite sensors by using information available from comparisons of those sensors with each other and with a reference through 'match-ups': occasions when the different sensors saw the same scene at the same time due to satellite overpasses. We explicitly include the + 0 term in the measurement equation to highlight the inbuilt assumptions. Here, for example, the equation includes a quadratic nonlinearity, but

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are assuming there are no higher nonlinearities; we are also making assumptions of sufficient monochromaticity as many terms are band-integrated quantities.

3. Uncertainty effects and correlation structures

The measurement equation, Eq.(1), describes the Level 1 product (here radiance) for a particular image pixel. Each term in the measurement equation is sensitive to a number of uncertainty effects.

Each of these effects has an associated uncertainty and will give rise to an unknown error, which can be considered a draw from a probability distribution whose standard deviation is given by the standard uncertainty. While the error itself cannot be known, we can say something about the error correlation between the measured Earth radiance values in different pixels of a satellite sensor image, or between different spectral bands on the satellite sensor. Independent random effects will cause errors which can never be corrected for in a single measured value, even in principle, because the effect is stochastic. In EO, a common example of a random effect is radiometric noise. In the laboratory, the uncertainty associated with random effects is usually determined by calculating the standard deviation of values from repeated measurements. For Earth observations, this method is only available for onboard calibration references and the noise for Earth scenes must be deduced from these calibration measurements and an understanding of the physics of the sensor.

Not all random effects are independent. Structured random effects arise in EO when effects are random, but have predictable patterned relationships across a set of measurements, perhaps because values of the effects are common for multiple pixels. An example is a cross-track sensor for which calibration measurements against a reference target is performed once per scanline. Any random effects associated with the derived calibration affect all Earth observations in that scan and therefore provide a common error to all those pixels.

Systematic effects are those that could in principle be corrected for, if sufficient knowledge about the effect were to be available, although even after any correction there is always some residual systematic error that remains that is unknown and quantified only by its associated uncertainties. These systematic effects cause errors that can be related across multiple measurements, perhaps for a whole mission. For example an error in the measurement of the instrument spectral response function will affect the analysis of all measurements by that sensor, though not in the form of a simple bias.

Because FCDRs are processed to produce CDRs (Level 2) by combining results from different spectral bands, and gridded-CDRs (Level 3) through the spatial and/or temporal combination of values in different pixels, it is important to determine the error-correlation structure between spectral bands and between different pixels. Note that the error correlation structure can be different in different dimensions. For example, a structure random effect caused by a calibration performed once per scanline, will be fully correlated between any two pixels within a scanline, but uncorrelated between any two pixels in different scanlines. Similarly an effect that depends on mirror angle may be fully correlated for pixels in the same relative position in all scanlines, but uncorrelated from one pixel to another within a scanline. For low Earth orbit satellites with across-track scanning (sensors that observe the Earth scanline by scanline as the satellite passes along a track), the most sensible dimensions over which to consider error correlations are within a scanline, from scanline to scanline and from orbit to orbit. Separately we must consider the correlation structure from channel to channel.

3.1. Error correlation forms

Error correlation occurs when there is a common error between two observations (in different spectral bands and/or in different spatial/temporal positions). In general, the error correlation form can be determined by considering the pattern for the common error. While there may be a large number of possible error correlation forms, we have defined a small subset which we consider sufficient for representing most practical cases for satellite sensors. Note that a particular effect may have a different correlation structure in different dimensions, as given above.

The "independent random" correlation represents the simplest case, when there is no error correlation for any pair of measured values (in the dimension of interest). A common example is noise on the Earth pixel count.

The "rectangular absolute" correlation is an error correlation form where there is a common error over a range of values defined in an absolute sense. A fully systematic effect would have a rectangular absolute correlation structure of infinite range. A finite range would represent a situation where a common error affects the measured values for a finite number of pixels. For example, if a single calibration value is obtained and used for all measurements within a particular time period, or for a certain number of scanlines, and this calibration value is then replaced with a refreshed value for a subsequent time period or set of scanlines, then there is a full correlation between values for pixels within that calibration period, and no correlation between values for pixels from one calibration period to the next.

The "triangular relative" correlation is an error correlation that arises from a running average with equal weights. If, for example, a calibration obtained once per scanline is averaged in a simple running average over a certain number of scanlines before and after the considered scanline, then the error correlation structure from one scanline to another would depend on the number of common calibrations. This provides a triangular correlation structure from scanline to scanline with the full base equal to twice the number of scanlines averaged. (Note that in this example, the correlation structure from pixel to pixel within the scanline is a rectangular absolute, across the whole scanline).

The "bell-shaped relative" correlation is an error correlation that occurs from a weighted average with a larger weight applied to the central value. The correlation structure can be considered as the convolution of two functions represented by the weights assigned to the rolling average. For a triangular weighting function this takes the form of a cubic spline over the overlap range (full base equal to twice the number of scanlines involved in the average). This cubic spline is sufficiently close to a Gaussian distribution in shape that we have represented a "bell-shaped relative" as a truncated Gaussian shape. For weights other than a triangle, the bell-shape is also likely to be sufficiently represented by a truncated Gaussian shape. This error correlation structure can also represent effects where we have very little information but the recognition that points closer in space/time are more correlated than those further away.

Within the FIDUCEO project we have developed a framework for formally coding this information, intend to be stored computationally in NetCDF files, this will be discussed further in future work.

3.2. Propagation of uncertainties

3.2.1. Uncertainties for a single pixel of an FCDR

In most cases we can consider each effect as independent of other effects. That means that the only covariance we need to consider for determining the Earth radiance of a single pixel (the FCDR quantity), is the covariance associated with the different harmonisation coefficients (see Section 2.2). Therefore we can write the Law of Propagation of Uncertainty [3] as

$$u^2\left(L_{\mathrm{E}}\right)=\sum_{i=1}^{n}\left(\frac{\partial L_{\mathrm{E}}}{\partial x_i}\right)^2 u^2\left(x_i\right)+\sum_{j=1}^{m}\left(\frac{\partial L_{\mathrm{E}}}{\partial a_j}\right)^2 u^2\left(a_j\right)+2\sum_{j=1}^{m-1}\sum_{k=j}^{m}\left(\frac{\partial L_{\mathrm{E}}}{\partial a_j}\right)\left(\frac{\partial L_{\mathrm{E}}}{\partial a_k}\right)u\left(a_j,a_k\right) \quad (2)$$

where the first term relates to the effects in the effects table, added in quadrature (the sensitivity coefficients and uncertainties are given in the effects tables); the second term relates to the uncertainty associated with each harmonisation coefficient; and the third term relates to the covariance of the harmonisation coefficients. Note that currently this level of uncertainty propagation is not undertaken at the radiance level for most if not all satellite products.

3.2.2. Error covariance for different channels in a single pixel

Often for the establishment of a CDR (climate data record of a geophysical parameter) from an FCDR (Earth radiance values used for CDR generation) the measured values in different spectral channels are combined. Therefore it is necessary to determine the error covariance between the Earth radiance values obtained for a single pixel in multiple spectral channels, and to provide a correlation matrix, $\boldsymbol{R}$, representing, for that effect, what is the correlation between channels. This matrix will often, but not always, be either the identity matrix or a matrix having unity in every element depending on whether an effect is common from channel to channel or has an independent error from channel to channel. Note that this is different from the error correlation structures describing pixel-to-pixel correlation, see following section.

For each effect in turn, we can consider the error covariance matrix for Earth radiance between channels due that that effect, to be the matrix multiplication of simple matrices, each square with a dimension equal to the number of channels. The matrix $\boldsymbol{C}_k$ has the sensitivity coefficients for each channel's Earth radiance to the quantity of the effect down the diagonal (and zero values elsewhere). The matrix $\boldsymbol{U}_k$ has the standard uncertainties associated with the effect (in units of the quantity) down the diagonal, and zeroes elsewhere. Note that for effects that are correlated between channels, this will be the same value down all elements of the diagonal, for effects that are not correlated between channels, it may have a different value down each element of the diagonal. The matrix $\boldsymbol{R}_k$ is the channel-to-channel correlation matrix for this effect. The covariance matrix for Earth radiance from channel-to-channel due to a single effect is given by a multiplication of these matrices.

As an example, consider the situation with three spectral channels that are all calibrated with the same onboard blackbody calibrator (ICT). The unknown error in the temperature of that blackbody, a draw from the probability distribution described by the uncertainty associated with the blackbody temperature, will be a common error for all three channels. Therefore the matrix $\boldsymbol{R}_i$ is a full matrix of ones. The $\boldsymbol{V}_i$ has the standard uncertainties associated with temperature down the diagonal (say 10 mK) and the $\boldsymbol{C}_i$ matrix has the sensitivity coefficient of each channel's Earth radiance ($L_{\mathrm{E},c}$) to the uncertainty associated with temperature, which will likely be calculated in a chain rule as the partial derivative of Earth radiance with respect to the calibration target radiance and the partial derivative of the ICT radiance with respect to temperature: $\frac{\partial L_{\mathrm{E},c}}{\partial T} = \frac{\partial L_{\mathrm{E},c}}{\partial L_{\mathrm{ICT},c}} \frac{\partial L_{\mathrm{ICT,c}}}{\partial T}$. Thus

$$\boldsymbol{C}_T \boldsymbol{U}_T \boldsymbol{R}_T \boldsymbol{U}_T^{\mathsf{T}} \boldsymbol{C}_T^{\mathsf{T}} = \begin{pmatrix} \frac{\partial L_{\mathrm{E},1}}{\partial T} & 0 & 0 \\ 0 & \frac{\partial L_{\mathrm{E},2}}{\partial T} & 0 \\ 0 & 0 & \frac{\partial L_{\mathrm{E},3}}{\partial T} \end{pmatrix} \begin{pmatrix} u_T & 0 & 0 \\ 0 & u_T & 0 \\ 0 & 0 & u_T \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} u_T & 0 & 0 \\ 0 & u_T & 0 \\ 0 & 0 & u_T \end{pmatrix}^{\mathsf{T}} \begin{pmatrix} \frac{\partial L_{\mathrm{E},1}}{\partial T} & 0 & 0 \\ 0 & \frac{\partial L_{\mathrm{E},2}}{\partial T} & 0 \\ 0 & 0 & \frac{\partial L_{\mathrm{E},3}}{\partial T} \end{pmatrix}^{\mathsf{T}} . \quad (3)$$

As another example, for the noise in the Earth counts, which is an effect with no channel-to-channel error correlation, for the central matrix $\boldsymbol{R}_k$ will be a diagonal matrix with 1s down the diagonal and zeroes elsewhere and the matrix $\boldsymbol{U}_k$ would be in units of Earth counts and give the uncertainty for each channel due to noise (which may be different channel to channel).

The covariance matrix for Earth radiance from channel-to-channel due to all effects is given by summing these covariance matrices, thus:

$$\boldsymbol{S}_c = \sum_k \boldsymbol{C}_k \boldsymbol{U}_k \boldsymbol{R}_k \boldsymbol{U}_k^{\mathsf{T}} \boldsymbol{C}_k^{\mathsf{T}} . \quad (4)$$

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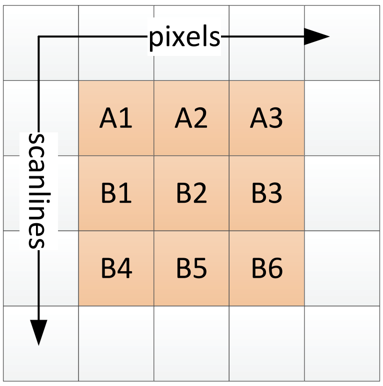
3.2.3. Error covariance between spatial pixels

When data processing requires combining data from different spatial pixels, for example to give regional spatial averages, we need to determine the error covariance between the Earth radiance values in different pixels. This can be determined in a similar manner to the error covariance between channels. For each effect, three matrices are needed for the sensitivity coefficients, standard uncertainties and correlation coefficients. These are square matrices with dimension equal to the number of pixels considered. The correlation matrix $\boldsymbol{R}_k$ will express the error correlation structure for the effect and will depend on both the correlation form, discussed above, and the separation of the pixels being considered, in each of the dimensions for correlation. So, for example, if we consider that the calibration process is averaged with a rolling average over three scanlines (the current one and one either side), then the error correlation between two pixels in the same scanline due to the calibration process is 1, and the error correlation between two pixels in neighbouring scanlines is 2/3 (two scanlines in common in averaging), and the error correlation between two pixels two scanlines apart is 1/3. This means that if we have a process that averages over nine pixels, as in Figure 1, then the error correlation, due to the uncertainty associated with that rolling-averaged calibration process, between pairs of pixels is 1, 2/3 or 1/3 depending on whether they are in the same scanlines, neighbouring scanlines or scanlines further apart.



$$\boldsymbol{R}_k = \begin{array}{cc} & \begin{array}{ccccccccc} \text{A1} & \text{A2} & \text{A3} & \text{B1} & \text{B2} & \text{B3} & \text{C1} & \text{C2} & \text{C3} \end{array} \\ \begin{array}{c} \text{A1} \\ \text{A2} \\ \text{A3} \\ \text{B1} \\ \text{B2} \\ \text{B3} \\ \text{C1} \\ \text{C2} \\ \text{C3} \end{array} & \begin{bmatrix} 1 & 1 & 1 & 2/3 & 2/3 & 2/3 & 1/3 & 1/3 & 1/3 \\ 1 & 1 & 1 & 2/3 & 2/3 & 2/3 & 1/3 & 1/3 & 1/3 \\ 1 & 1 & 1 & 2/3 & 2/3 & 2/3 & 1/3 & 1/3 & 1/3 \\ 2/3 & 2/3 & 2/3 & 1 & 1 & 1 & 2/3 & 2/3 & 2/3 \\ 2/3 & 2/3 & 2/3 & 1 & 1 & 1 & 2/3 & 2/3 & 2/3 \\ 2/3 & 2/3 & 2/3 & 1 & 1 & 1 & 2/3 & 2/3 & 2/3 \\ 1/3 & 1/3 & 1/3 & 2/3 & 2/3 & 2/3 & 1 & 1 & 1 \\ 1/3 & 1/3 & 1/3 & 2/3 & 2/3 & 2/3 & 1 & 1 & 1 \\ 1/3 & 1/3 & 1/3 & 2/3 & 2/3 & 2/3 & 1 & 1 & 1 \end{bmatrix} \end{array}$$

Figure 1 (left): A representation of nine pixels that are combined in a regional average, (right) the form of the correlation coefficient matrix for an effect that is based on a rolling average over 3 scanlines, e.g. from a common calibration process. The correlation coefficient matrix has a dimension 9 × 9 representing the different pixels. The error due to this calibration as a correlation of 1 for pixels within the same scanline (sharing all three calibration points), of 2/3rds for pixels in neighbouring scanlines (sharing two of three calibration points) and of 1/3$^{\text{rd}}$ for pixels two scanlines apart, sharing 1 of 3 calibration points.

This would be multiplied by the diagonal matrix $\boldsymbol{U}_k$ representing the uncertainties associated with the calibration in each of the nine pixels, and the diagonal matrix $\boldsymbol{C}_k$ giving the sensitivity coefficient for the Earth radiance in each of the nine pixels to the calibration. Other error effects will have a different correlation structure, and overall the error covariance for Earth radiance for the set of pixels will be obtained by adding together the error covariance matrices for each effect, thus:

$$\boldsymbol{S}_p = \sum_k \boldsymbol{C}_k \boldsymbol{U}_k \boldsymbol{R}_k \boldsymbol{U}_k^{\mathrm{T}} \boldsymbol{C}_k^{\mathrm{T}} \ . \tag{5}$$

3.2.4. Propagation to CDRs

A CDR is determined from an FCDR through a processing step that combines information from the FCDR (measured radiance values in each Earth pixel, potentially combining different spectral bands), with external information about the environmental state. While uncertainties associated with the additional information must be considered separately, the uncertainties from the FCDR can be straightforwardly propagated using the Law of Propagation of Uncertainty together with the error covariance information described above. Where a CDR is gridded in time or space (i.e. averaged over an area and/or time), the information about pixel-to-pixel error covariances must be included to obtain the correct uncertainties.

4. Harmonisation of the measurement equation

The harmonisation coefficients (the a_i in Eq.(1)) are determined through a regression analysis using sensor-to-sensor match-ups for different pairs of sensors in the series (creating a chain from the present day to the first satellite launched) and, where a suitable reference is available, from at least one sensor in that chain to a suitable independent reference, solving simultaneously the calibration parameters for all sensors in the series, connected through a set of match-ups between pairs of sensors.

The harmonisation problem is a multi-parameter, non-linear least-squares regression problem, with a very large data set (typically, hundreds of millions of match-ups), where there are error correlations between data relating to different match-ups, and where there are uncertainties for all measured variables. Solving this regression problem requires an "Errors in Variables" approach that can handle the full correlation structure and is a subject of ongoing scientific research that will be reported in a later publication.

The process of harmonisation will provide the harmonisation coefficients (the a_i) and the associated error covariance matrix; because the coefficients are determined from the same set of data, there will be an error covariance term associated with each pair of coefficients.

5. Conclusions

In this paper we have introduced some key principles for the application of metrological techniques to historical satellite sensors and the FCDRs and CDRs. Within the European project FIDUCEO we are currently developing full analyses for four different FCDRs in the visible, thermal infrared and microwave spectral regions. The process undertaken for this analysis has been described.

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